

Giant mass and anomalous mobility of particles in a fermionic system

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We calculate the mobility of a heavy particle coupled to a Fermi sea within a non-perturbative approach valid at all temperatures. The interplay of particle recoil and of strong coupling effects, leading to the orthogonality catastrophe for an infinitely heavy particle, is carefully taken into account. We find two novel types of strong coupling effects: a new low energy scale T^* and a giant mass renormalization in the case of either near-resonant scattering or a large transport cross section σ . The mobility is shown to obey two different power laws below and above T^* . For $\sigma \gg \lambda_f^2$, where λ_f is the Fermi wave length, an exponentially large effective mass suppresses the mobility.

Some remarkable advances in condensed matter physics are based on a thorough analysis of models of a single impurity coupled to a many-particle system. The polaron problem and the mobility of ions in liquid ^3He are well-known examples for the dynamical behavior of a delocalized particle in a bosonic or fermionic bath, respectively. We will consider the latter case of a delocalized but heavy particle strongly interacting with a Fermi liquid.

Concerning the experimental context, a $^3\text{He}^+$ -ion in normal-fluid ^3He is the cleanest possible heavy-particle Fermi-liquid system. Unfortunately, the transition to the superfluid state cuts off the available low-temperature range [1]. The particle is indeed heavy and of large cross section since the ion forms a snowball: about 100 Helium atoms (depending on pressure) are tightly bound at temperatures T up to several hundred mK. Other real fermionic systems, such as muons in metals or valence band holes in n -type doped semiconductors, show a more complex dynamical behavior, usually involving several diffusion mechanisms [2–5]. Nevertheless, our approach is supposed to be valid in the low- T regime.

We will discuss two strong coupling effects of a heavy particle [6,7] in a fermionic bath, both of which have not been reported before, basically because a microscopic strong coupling calculation of the mobility has not been developed for low temperatures. As to the origin of strong coupling effects we actually have to distinguish two scenarios: (1) the scattering phase at the Fermi energy of bath particles is close to $\delta = \pi/2$ in any single scattering channel; (2) the transport cross section σ of the heavy particle is large: $\sigma \gg (2\pi/k_f)^2$. Obviously, each of the two scenarios implies a strong coupling of bath particles to the impurity.

In the first scenario we work close to a resonance at the Fermi energy. This may signify that an attractive channel exists with sufficiently large binding energy. Alternatively, we may consider a strong enough repulsive interaction between the particle and the fermionic bath, e.g. the Hubbard model in the spin-polarized sector with

one overturned spin which interacts with the free Fermi system of up-spins through a local interaction U . If the tight-binding band is nearly half-filled with up-spins and the repulsive interaction approaches infinity, $U \rightarrow \infty$, the bath particles at the Fermi energy encounter a phase shift close to $\pi/2$. These problems cannot be solved within perturbation theory. Indeed, the heavy-particle mobility changes its temperature dependence drastically with respect to the perturbational limit if the phase shift exceeds a minimal value in at least one channel: the temperature (and frequency) power law behavior acquires an anomalous exponent as we will demonstrate.

The second scenario may be encountered already for relatively small phase shifts in each of the scattering channels provided the particle couples to the bath through a sufficiently large number N of channels. We find that the effective mass of the particle is tremendously increased for low T : it scales with an exponential function, the exponent of which is proportional to a power of N .

The mobility of a heavy particle in a fermionic environment has been investigated for more than three decades [1,8,4,5]. Concerning translational invariant systems, as ions in ^3He , the work by Wölfle et al. summarized the previous findings and presented the first unified treatment for all temperature ranges below the Fermi temperature within a self-consistent Mori-Zwanzig scheme. The approach is phenomenological and cannot account for part of the strong coupling effects discussed here. More recently Prokof'ev [9] put forward a microscopic path integral scheme, yet his evaluation is restricted to the high temperature corrections in the mobility.

The basis of our evaluation (for space dimension $d > 1$) is an effective low-energy action for the heavy particle, first introduced by Sols and Guinea [10], investigated in more detail by Prokof'ev [9], and evaluated for the heavy-particle spectral function in a previous paper [11]:

$$S_{\text{eff}} = S_o - \frac{1}{2} \iint_0^\beta d\tau d\tau' \mathcal{F}(|\mathbf{R}(\tau') - \mathbf{R}(\tau)|) \rho(\tau' - \tau). \quad (1)$$

The first term on the rhs is the action for a free particle, $S_o = \frac{1}{2} \int_0^\beta d\tau M_o \dot{\mathbf{R}}(\tau)^2$, and $\mathcal{F}(|\mathbf{R}' - \mathbf{R}|)$ is determined through the overlap of the electronic ground state $\phi_{\mathbf{R}}$ with particle at position \mathbf{R} and a state $\phi_{\mathbf{R}'}$ in the thermodynamic limit $N_e \rightarrow \infty$ [12]: $\langle \phi_{\mathbf{R}'} | \phi_{\mathbf{R}} \rangle \rightarrow \exp\{-[(\delta/\pi)^2 - \mathcal{F}(|\mathbf{R}' - \mathbf{R}|)] \log N_e\}$ where

$$\mathcal{F}(|\mathbf{R}|) = (\delta/\pi)^2 - \frac{1}{\pi^2} \arcsin^2(\sqrt{1-x^2} \sin \delta) \quad (2)$$

with $x = \langle e^{i\mathbf{k}\mathbf{R}} \rangle_{|\mathbf{k}|=k_f}$ (see Fig. 1). These relations apply for *s*-wave scattering with phase shift δ . Generalizations for several scattering channels are found in the literature [12,13]. The leading low-energy form of $\rho(\tau - \tau')$ in $d > 1$ [14] is $\rho(\tau - \tau') = (\pi/\beta) \sum_{n \neq 0} |\omega_n| e^{i\omega_n(\tau - \tau')}$ which reflects that the number of virtual excitations close to the Fermi surface is proportional to ω . This behavior and the Friedel oscillations of $\mathcal{F}(R)$ are rooted in the fermionic character of the bath.

Alternatively, one could set up a Hamiltonian for both, the heavy particle (\mathbf{P}, \mathbf{R}) and the fermionic degrees of freedom ($c_{\mathbf{k}}^\dagger, c_{\mathbf{k}}$)

$$H = \frac{\mathbf{P}^2}{2M_o} + \sum_{\mathbf{k}} \frac{k^2}{2m} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + U \sum_{\mathbf{kk}'} e^{i(\mathbf{k}' - \mathbf{k})\mathbf{R}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}'} \quad (3)$$

for *s*-wave scattering. In a second step, the fermions are traced out. This procedure results in an effective heavy-particle action which involves any number of retardations (i.e. time integrals) and it cannot be handled further except for a few limiting cases. Fortunately, the effective action (1) reproduces all exactly known limits of this more basic approach: the spectral function of the heavy particle was evaluated and discussed in this respect [11], and the mobility $\mu(T)$ is identical in both approaches in the exactly known high-temperature limit: a constant behavior $\mu(T) = \mu_o = e/(M_o \Gamma)$ plus logarithmic corrections [9,11]. Here $\Gamma = nk_f \sigma / M_o$ is the scattering rate, $k_f = 2\pi/\lambda_f$ the Fermi wave vector and n the particle density.

The success of the approach based on the effective action (1) is actually not surprising. It correctly accounts for the two competing effects which control the dynamics: the orthogonality catastrophe (OC) through the exact form of the overlap and the recoil through translational invariance. The relevant low-energy scale is supposed to settle which of the two effects dominates. It may be anticipated that the maximum recoil energy $E_R = (2k_f)^2/2M_o$ transferred in a collision process is the relevant energy scale. For frequency ω or temperature T far above E_R the energy balance in scattering processes is independent of the recoil—i.e. physics is governed by the $\mathbf{R} = 0$ saddle point and the corresponding fluctuations: the high- T mobility results from the coefficient of the R^2 -term in $\mathcal{F}(R) = (\delta/\pi)^2 - (\Gamma M_o/2\pi) R^2 + O(R^4)$.

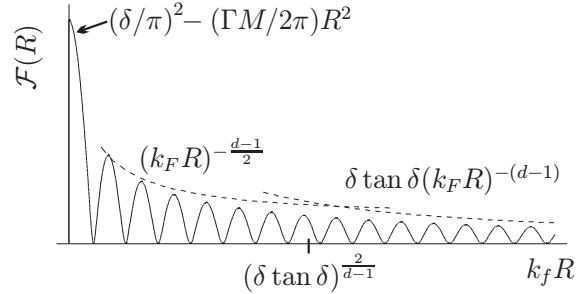


FIG. 1. Qualitative behavior of $\mathcal{F}(R)$ for strong coupling.

For frequencies or temperatures much less than E_R the available phase space for scattering processes with momentum transfer $|\Delta\mathbf{k}| \simeq 2k_f$ is restricted by recoil, i.e. in d dimensions by a factor $(T/E_R)^{(d-1)/2}$ and we expect a well-defined quasi-particle for $T \rightarrow 0$ —albeit with renormalized mass or possibly coupling constant. For the mobility this corresponds to a $1/T^{(d+1)/2}$ power law which is the Fermi liquid behavior well known for many decades from weak coupling analysis [1]. It is instructive to realize that the decay of the envelope of the overlap function $\mathcal{F}(R)$ for $k_f R \gg 1$ determines the low temperature behavior: firstly, only a decaying envelope function results in a finite quasiparticle weight Z [11], and secondly, the long-range decay $\propto \delta \tan \delta / (k_f R)^{d-1}$ translates into the power-law behavior of the incoherent part of the spectral function and the mobility.

Here we want to investigate the significance of the second energy scale, the particle-bath interaction U . The cross section of the particle is directly related to the interaction via the phase shift δ : $nk_f \sigma = M_o \Gamma = E_R \sin^2 \delta / \pi d$. In phenomenological approaches it was always explicitly or implicitly assumed that the interaction enters $\mu(T)$ only through the cross section. However the phase shift may also lead to a subtle interference effect for the moving particle. This interference effect is encoded in the spatial decay of $\mathcal{F}(R)$ (cf. Fig. 1). It decays anomalously slow for $\delta \rightarrow \pi/2$: $\mathcal{F}(R) \propto 1/(k_f R)^{(d-1)/2}$ for $1 \ll k_f R \ll (\delta \tan \delta)^{2/(d-1)} \equiv k_f R_c$ whereas for larger R the envelope function decays with $1/(k_f R)^{d-1}$, as stated above. For $\delta = \pi/2$, the anomalous decay extends to $R \rightarrow \infty$. The cross-over length R_c corresponds to a new low-energy scale $E^* = E_R / (\delta \tan \delta)^{4/(d-1)}$ which approaches $E^* \rightarrow 0$ with $\delta \rightarrow \pi/2$ and which exists only for $\tan \delta \gg 1$, i.e. we consider a strong-coupling anomaly. This observation implies that physical quantities will behave differently for T (or ω) below or above E^* . Specifically, the power-law behavior above E^* is characterized by an anomalous exponent—as we will show for $\mu(T)$. A similar anomalous enhancement of interference effects near $\delta \simeq \pi/2$ may be relevant for other fermionic problems with dynamical scatterers at distinct spatial positions.

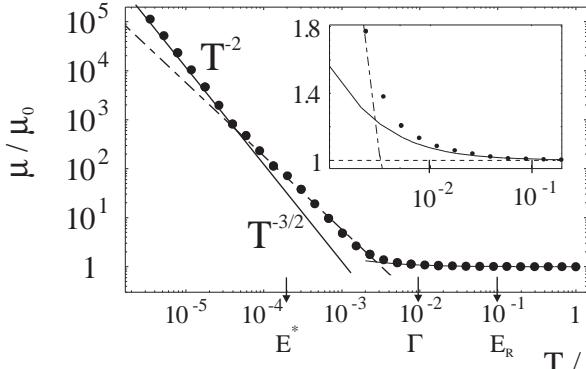


FIG. 2. $\mu(T)$ in the strong coupling regime with $\delta = 0.95\pi/2$, $\omega_c \simeq \epsilon_f$. The inset displays $\mu(T)$ on a linear scale together with the analytical result of the high- T expansion.

We evaluated the mobility in the simplest scheme available which still reproduces the exact high T behavior, including the non-perturbative logarithmic corrections. It also reproduces the Born-approximation results of the previous literature which are commonly agreed upon as to display the correct power-law behavior for the lowest temperature regime. Self-consistency is indispensable for a successful evaluation since a diffusing particle exhibits an entirely different long-time behavior as compared to a free particle. In order to tackle the mobility $\mu_{ij}(\omega) = -(1/i\omega) \langle \dot{R}_i \dot{R}_j \rangle_{(\omega+i0)}$ we have to examine a $\langle RR \rangle_S$ -correlator which is a path integral evaluated with action S (Eq. (1)). For this purpose we introduce a general quadratic action

$$S_V[A] = S_o - \frac{1}{4} \iint_0^\beta d\tau d\tau' A(\tau - \tau') \left(\mathbf{R}(\tau) - \mathbf{R}(\tau') \right)^2 \quad (4)$$

and expand the correlator to first order in $\Delta S = S - S_V$: $\langle RR \rangle_S = \langle RR \rangle_{S_V} - \langle (RR) \Delta S \rangle_{S_V} + \langle RR \rangle_{S_V} \langle \Delta S \rangle_{S_V} + O(\Delta S^2)$. The best possible action $S_V[A]$ to this order results from the condition that only the first term survives in next-to-leading order, i.e. $A(\tau)$ has to be found from $\langle (RR) \Delta S \rangle_{S_V} = \langle RR \rangle_{S_V} \langle \Delta S \rangle_{S_V}$. And the mobility is

$$\mu(\omega + i0, T) = \left[\frac{A(\omega + i0, T)}{i\omega} - i\omega M_o \right]^{-1} \quad (5)$$

where $A(\omega + i0, T)$ is the analytical continuation of the Fourier transform of $A(\tau)$. It is straightforward to show that this procedure is equivalent to Feynman's variational principal (FVP). The early FVP evaluations of the mobility in the polaron problem did not fully reproduce the weak coupling limit. However only few variational parameters were used to determine $A(\tau)$. These inconsistencies are repaired if the full function $A(\tau)$ is determined self-consistently. Details of this calculation will be presented in a more extended article. Fig. 2 displays the calculated the static $\mu(T)$ in $d = 3$. The phase shift is close enough to $\pi/2$ so that the anomalous behavior $\mu(T) \approx T^{-3/2}$ extends over two decades.

The second pronounced strong coupling effect, the giant mass renormalization, is illustrated most intuitively via a rough estimate based on a Kramers-Kronig relation. It relates mass $M(\omega)$ and the friction coefficient $\eta(\omega)$ as defined by the exact inverse mobility (at $T = 0$): $\mu(\omega + i0)^{-1} = \eta(\omega) - i\omega M(\omega)$. The friction $\eta(\omega)$ [15] attains its high energy value η' for frequencies larger than the relevant energy scale E_R (and below ϵ_f). For $\omega \ll E_R$ the phase space for scattering processes approaches 0 so that $\eta(\omega)$ converges algebraically to zero. The zero-frequency $T = 0$ mass enhancement is therefore estimated by a step-like $\eta(\omega)$: $\Delta M \propto \int_{E_R}^{\epsilon_f} d\omega \eta(\omega)/\omega^2 \simeq \eta'/E_R = (\eta'/E_R^{(o)}) \cdot (M_o + \Delta M)/M_o$. The index o refers to unrenormalized quantities. Since the friction coefficient is proportional to the cross section of the particle, or rather $\eta'/E_R^{(o)} \simeq M_o(k_f a)^2$ where a is the diameter of the particle, we find from this estimate that $\Delta M/M_o \sim (a/\lambda_f)^2/[1 - (a/\lambda_f)^2]$ which diverges for $a \sim \lambda_f$. While the divergence is an artifact of this estimate it nevertheless signals that the large number of virtual low energy excitations for $\omega \simeq E_R \ll \epsilon_f$ enhances the dynamical mass very effectively.

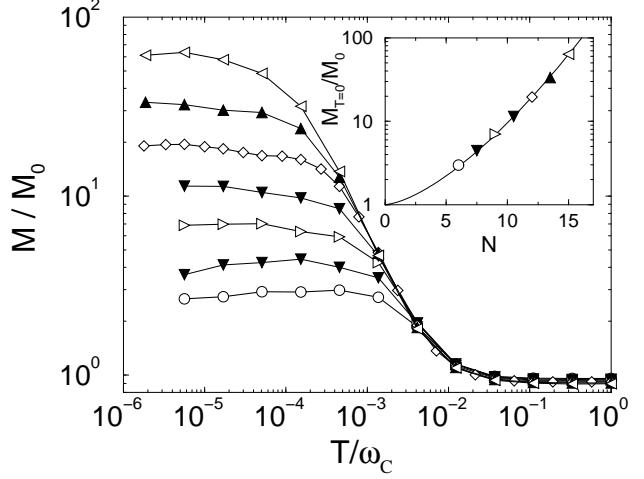


FIG. 3. Effective mass $M(T)$ for $M_o = 40m$ and $\delta = 0.95\pi/2$. The respective number of scattering channels is found by comparison with the inset which displays the low- T effective mass (the number of channels ranges from 6 to 15).

The T -dependent dynamical mass has to be calculated through the self-consistent scheme outlined above. We have to extend it for a large number of scattering channels in order to raise σ far beyond λ_f^2 . One may include more scattering channels by systematically generalizing $\mathcal{F}(R)$ as has been accomplished by Vladar [13] who included higher angular momentum channels N up to $N = 3$.

However we do not intend to model a specific scatterer. In this case, it is more practical to introduce a large number of spin channels to investigate this type of strong coupling effect in a generic way. The number of scattering channels then enters as a multiplicative factor in the

exponent of the overlap: $\mathcal{F}_N(R) \equiv N\mathcal{F}(R)$. Accordingly, the inverse high- T mobility scales with a trivial factor N : $\mu_{oN}^{-1} = N\mu_o^{-1}$ —and in leading order of perturbation theory ($\mathcal{F}_N(R) \ll 1$) this trivial dependence on N is valid down to $T \rightarrow 0$. The self-consistency, however results in a tremendous suppression of the low- T mobility (Fig. 4) and a giant increase of the zero-frequency effective mass (Fig. 3). The numerical analysis shows that

$$\frac{M_{T \rightarrow 0}}{M_o} \simeq \exp \left[c \left(\frac{\Gamma}{E_R^{(o)}} \right)^{3/2} \right], \quad \frac{\Gamma}{E_R^{(o)}} \sim \left(\frac{a}{\lambda_f} \right)^2 \gg 1 \quad (6)$$

is an excellent fit (Fig. 3, inset). The factor c depends weakly on the phase shift and is approximately $c \simeq 0.21$ in the perturbative regime and $c \simeq 0.68$ for $\delta = 0.95 \pi/2$.

An exponential increase of M/M_o is indeed expected from the requirement for a smooth transition from the high- T to the low- T regime: the high- T analysis yields for $\mu(T)$ a constant plus logarithmic corrections down to $T_s \simeq \Gamma \exp(c'\Gamma/E_R^{(o)})$ [8]. On the other hand, the low- T behavior is found analytically because self-consistency is not required: $\mu(T)^{-1} \simeq \pi^{-2} \delta \tan \delta \cdot M T (T/E_R)^{(d-1)/2}$. Assuming that low- and high- T expressions connect smoothly at T_s , we have to demand that $M_{T \rightarrow 0}/M_o \geq 2\Gamma/T_s \approx \exp(c'\Gamma/E_R^{(o)})$. This estimate does not yield the same exponent as the full numerical calculation but it supports the notion of an exponentially large mass.

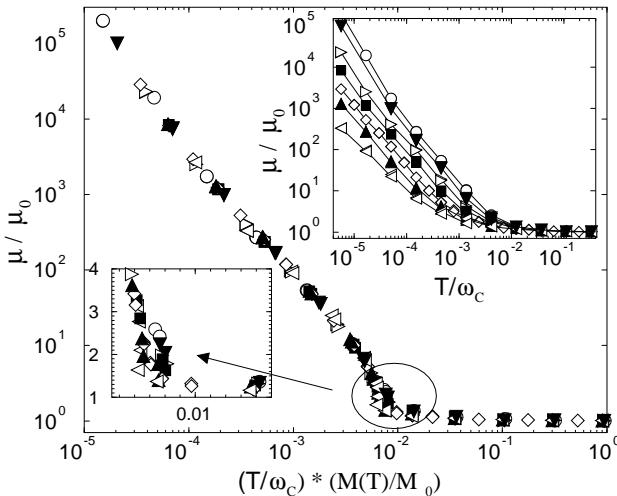


FIG. 4. Scaled mobility of the N -channel model for the same parameters as in Fig. 3. The upper inset displays the unscaled mobility (the highest mobility corresponds to 6 channels, the lowest to 15 channels implying a large cross section). The lower inset demonstrates that scaling fails for intermediate temperatures.

Also the mobility depends exponentially on the cross section as is displayed in the upper inset of Fig. 4. The low- T mobility, however, is explained entirely by the mass renormalization. Consequently, all curves of the upper inset collapse onto a single line for the lowest T . This is

not true for intermediate temperatures: the lower inset magnifies this non-universal regime.

The dramatic rise in the effective mass of large heavy particles should be clearly observable for ions in ^3He . While the superfluid transition will inhibit the observation of the low-temperature effective mass, we expect a large increase of the effective mass $\propto 1/T$ in the regime where a logarithmic increase of the mobility has been observed [16]. The experimental situation is more complex for muons in metals and will be discussed elsewhere. Our predictions are relevant in a regime where the temperature is low enough so that $\mu(T) > \mu_0$ holds where μ_0 is the mobility in the absence of a periodic potential (which can be determined from fits of the mobility to the Kondo-Yamada theory [4,5]). Unfortunately, all mobility experiments for muons in metals (even in aluminum) seem to be in the opposite regime $\mu(T) < \mu_0$ where the effect of the periodic potential determines the mobility. Therefore one either has to reach temperatures below 10mK in aluminum or find different metals with more mobile muons.

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